Machine Learning

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Contents

1 Introduction

1.1 What is Machine Learning

1. Machine Learning
    - Grew out of work in Artificial Intelligence (AI)
    - New capabilities for computers
2. Examples:
    - database mining
    - applications can't programby hand (handwriting recognition, Natural Language Processing (NLP), Computer Vision)
    - Neuromorphic applications
3. Definition
    - Arthur Samuel(1959)

        > Machine Learning: Field of study that gives computers the ability to learn without being explicitly programmed.

    - Tom Mitchell(1998)

        > Well-posed Learning Problem: A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.

4. Machine Learning in this course:
    (a) Suupervised Learning
    (b) Unsupervised Learning
    (c) Others: reinforcement learning, recommender systems
    (d) Practical application techniques

1.2 Supervised Learning

In supervised learning, the *the right answer* is given. For example:

1. Regression: predict real-valued output.
2. Classification: predict discrete-valued output.

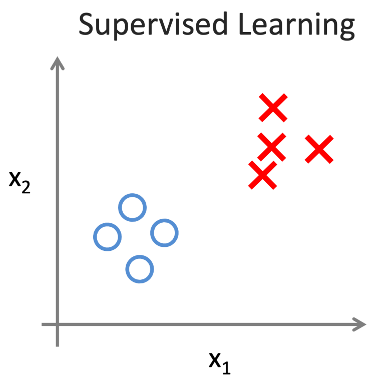


Figure 1: Supervised Learning

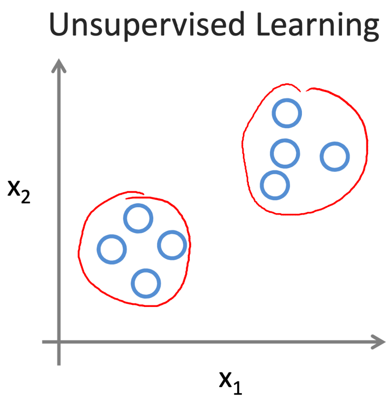


Figure 2: Unsupervised learning

1.3 Unsupervised Learning

The right answer is not given, e.g. cocktail problem (distinguishing two voices from an audio file.)

2 Linear Regression with One Variable

2.1 Model Representation

2.1.1 Notations

For a training set:

- **m** = Number of training examples.
- **x** = "input" variable / features.

- **y** = “output” variables / “target” variable.
- **(x,y)** - one training example.
- **($\mathbf{x^i}$,$\mathbf{y^i}$)** denotes the $\mathrm{i^{th}}$ training example

2.1.2 Hypothesis Function

A hypothesis function (h) maps input (x) to estimated output (y). How do we represent h?

$$\boxed{\textbf{Hypothesis Function} \quad h_\theta(x) = \theta_0 + \theta_1 x} \tag{1}$$

We can apply *Univariate linear regression* with respect to x.

2.2 Cost Function

Recall 1. The θ_is are parameters we have to choose. The intuition is is that we want to choose θ_i s such that h_θ is closest to y for our training examples (x,y).

$$\boxed{\textbf{Cost Function} \quad J(\theta_0, \theta_1) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2} \tag{2}$$

Summary

1. **Hypothesis** $h_\theta(x) = \theta_0 + \theta_1 x$
2. **Parameters** θ_0, θ_1
3. **Cost Function** $J(\theta_0, \theta_1) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$
4. **Goal** $\min_{\theta_0,\theta_1} J(\theta_0, \theta_1)$

2.3 Gradient Descent

2.3.1 Intuition

1. We have some function $J(\theta_0, \theta_1)$, we want to $\min_{\theta_0,\theta_1} J(\theta_0, \theta_1)$
2. Outline: start with some θ_0, θ_1, keep changing θ_0, θ_1 to reduce $J(\theta_0, \theta_1)$ until we end up at a minimum.

2.3.2 Gradient Descent Algorithm

Algorithm

repeat until convergence{

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \quad \text{(for j=0 and j=1).}$$

}

Notes

1. the := denotes non-blocking assignment, i.e. simultaneously updates $\theta_0 and \theta_1$
2. We use the derivative to find a local minimum.
3. α denotes the learning rate. Gradient descent can converge to a local minimum even when the learning rate α is fixed. As we approach a local minimum, gradient descent will automatically take smaller steps. Therefore it is not needed to decrease α over time.

2.3.3 Gradient Descent with Linear Regression

Recall, we have:

1. Gradient Descent Algorithm:

   repeat until convergence{

   $$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \quad \text{(for j=0 and j=1).}$$

   }

2. Linear Regression Model:

   $$h_\theta(x) = \theta_0 + \theta_1 x$$

   $$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

   We can substitute the above equations, which gives us:

   $$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})$$

   $$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

3 Review of Linear Algebra

This is section is a basic review of linear algebra. I have skipped this section for now and will come back to it if time permits.

4 Linear Regression with Multiple Variables

4.1 Multiple features

Recall in the single variable case, we have a single input (x), two parameters(θ_0, θ_1). The hypothesis can be expressed as:

$$h_\theta(x) = \theta_0 + \theta_1 x.$$

Now, consider a generalized case where there are multiple features: X_1, X_2, X_3. The information can be organized in a table with example numerical values:

Sample Number (i)	X_1	X_2	y
1	6	87837	787
2	7	78	5415
3	545	778	7507
4	545	18744	7560
5	88	788	6344

Table 1: Sample Table

From Table 1, one can see that each row is a sample a feature on each column.

4.1.1 Notation

1. **n**: number of features.
2. $\mathbf{x^{(i)}}$: (row vector) input features of the i^{th} training example. i= 1, 2,. . . , m.
3. $\mathbf{x^{(i)}}_\mathbf{j}$: value of feature j in the i^{th} training example. j= 1, 2, . . . , n.

4.1.2 Hypothesis

Previously,

$$h_\theta(x) = \theta_0 + \theta_1 \cdot x$$

Now, we can extend the hypothesis to :

$$h_\theta(x) = \theta_0 \cdot 1 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2$$

For convenience of notation, let's define x_0=1, i.e. $\mathrm{x^i}_0$=1 $\forall$ i.

Therefore, we have: $\mathbf{x}=\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$ and $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$. Then, the hypothesis function can be written as:

$$\begin{aligned} h_\theta(x) &= \begin{bmatrix} \theta_0 & \theta_1 & \theta_2 & \dots & \theta_n \end{bmatrix} \cdot \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \\ &= \theta^T \cdot \mathbf{x} \end{aligned} \tag{3}$$

This is *Multivariate linear regression.*

4.2 Gradient Descent for Multiple Variables

4.2.1 Algorithm

Summary for Multivariables

1. **Hypothesis** $h_\theta(x) = \theta^T \cdot \mathbf{x}$
2. **Parameters** θ
3. **Cost Function** $J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$
4. **Goal** $\min_\theta J(\theta)$

Gradient Descent for Multiple Variables

repeat until convergence {

$$\theta_j := \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta) \qquad \text{(for j=0, 1,\dots n)}$$

}

$$\theta_j := \theta_j - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(\mathbf{x}^{(\mathbf{i})}) - y^{(i)}) \cdot x_j^{(i)}$$

Note: $x_0^{(i)} = 1$, by definition.

4.2.2 Vectorized Implementation

One can work out the linear algebra and arrive at the following simplification using vectorized operations. The cost function J can be expressed as:

$$J(\theta) = \frac{1}{2m}(\mathbf{X}\theta - \mathbf{y})^T(\mathbf{X}\theta - \mathbf{y}) \tag{4}$$

The MATLAB implementation is as follows:

```
m = length(y); % calculate how many samples
J = 1/(2*m)*((X*theta-y).')*(X*theta-y);
```

Gradient descent can be vectorized in the form:

$$\theta = \theta - \frac{\alpha}{m} \cdot \mathbf{X}^T \cdot (\mathbf{X}\theta - \mathbf{y}) \tag{5}$$

The MATLAB implementation is as follows:

```
m = length(y); % number of training examples
for iter = 1:num_iters
    theta = theta - alpha/m* X.'*(X*theta -y);
```

4.3 Gradient Descent in Practise I: Feature Scaling

- Idea: ensure each featurre are on a similar scale
- Get every feature into approx. $-1 \leq x_i \leq 1$($\sim$ order)
- **Mean Normalization**: Replace x_i with $\frac{x_i - \mu_i}{s_i}$, where μ_i and s_i are the sample mean and standard deviation, respectively.

4.4 Gradient Descent in Practise II: Learning Rate

- Ensure gradient descent is working: plot J_θ over each number of iteration (not over θ !)
- Example automatic convergence test: for sufficiently small α J_θ should decrease by less than 10^{-3} i one iteration.
- If α is too small, gradient descent can be slow to converge.
- If α is too large, gradient descent may not converge.
- To choose α, try 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1... (by 3x)

4.5 Features and Polynomial Regression

We can fit into different polynomials by choice, using multivariate regression. Recall

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

Let x_1 be x^1, x_2 be x^2, x_3 be x^3. Note we should still apply feature scaling to x_1, x_2, and x_3 individually!

4.6 Normal Equation

The normal equation provides a method to solve for θ analytically. For our data with m samples, n features, recall each sample can be written as:

$$\mathbf{x^{(i)}} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_j^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}$$

We can construct a design matrix:

$$\mathbf{X} = \begin{bmatrix} — & (x^{(1)})^T & — \\ — & (x^{(2)})^T & — \\ — & (x^{(3)})^T & — \\ & \vdots & \\ — & (x_m^T & — \end{bmatrix} \tag{6}$$

Then θ can be found by the normal equation:

$$\theta = (\mathbf{X^T X})^{-1}\mathbf{Ty} \tag{7}$$

Normal equation is useful as no α is required to and we do not need to iterate. However, we do have to compute $(X^T X)^{-1}$, which can be computationally expensive when n is large. The complexity is O(n^3) for inverse operations. Gradient Descent is useful when n is large (many features).

4.7 Normal Equation and Non-invertibility

What if $(X^T X)^{-1}$ is non-invertible?

- Redundant features (linearly dependent), i.e. having same information in two different units.
- Too many features (i.e. m $\leq$ n). Delete some features or use regularization

5 Octave/MATLAB Tutorial

6 Logistic Regression

6.1 Classification

- Binary Classification: y $\in \{0, 1\}$, where 0 denotes the negative class; 1 denotes the positive class.

- Multi-class Classification:y $\in \{0, 1, \cdots, n\}$

We will be using binary classification:

- Linear regression is not suitable for classification: since $h_\theta(x)$ can output out of range, i.e. < 0 or > 1.
- We will use **logistic regression**, which ensures that the output $h_\theta(x)$ is between 0 and 1.

6.2 Hypothesis Representation

6.2.1 Logistic function

The idea is to have $0 \le h_\theta(x) \le 1$. Instead of the linear regression hypothesis: $h_\theta(x) = \theta^T x$, we will let:

$$h_\theta(x) = g(\theta^t x),$$

where

$$g(z) = \frac{1}{1 + e^{-z}}$$

g(z) is known as the **logistic function**, also known as the Sigmoid function. Figure 3 shows a plot of the logistic function, which ranges from 0 to 1.

which yields

$$h_\theta(x) = \frac{1}{1 + e^{-z}} \tag{8}$$

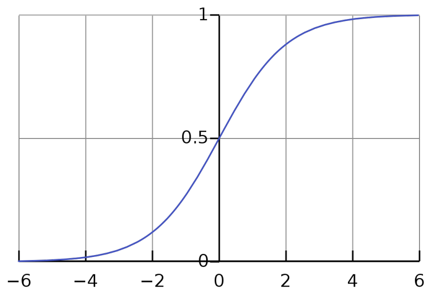


Figure 3: Sigmoid Function

6.2.2 Interpretation of Hypothesis Output

$h_\theta(x) =$ estimated probability that y$=$ 1 on input x. For example, $h_\theta(x) = 0.7$ gives us a probability of 70% that are output is 1. From a probability theory point of view, one can express $h_\theta(x)$ as $P(y = 1 \mid x; \theta)$.

Note that since this is a probability and the total probability sums up to 1, and the real y can only be either 0 or 1:

$$P(y = 0 \mid x; \theta) + P(y = 1 \mid x; \theta) = 1$$

6.3 Decision Boundary

Recall so far we have $h_\theta(x) = g(\theta^T x)$ and $g(z) = \frac{1}{1+exp(-z)}$. Suppose we set $h_\theta(x) = 0.5$ to be our determining factor for whether y= 0 or y =1. Note that from 3, one can observe that $h_\theta(x) = 0.5$ corresponds to $\theta^T x = 0$, which is the **decision boundary**. The decision boundary is the equation which separates the different classes on a plot. There are linear and non-linear decision boundaries.

6.4 Cost function

Previously, we had $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} Cost(h_\theta(x^{(i)}), y^{(i)})$, where $Cost(h_\theta(x), y) = \frac{1}{2}(h_\theta(x) - y)^2$. Now, the definition of the hypothesis h_θ has changed to $\frac{1}{1+exp(-\theta^T x}$, as a result the cost function is now non-convex.

Logistic Regression Cost Function
Therefore, a new cost function definition is needed. We propose:

$$Cost(h_\theta(x), y) = \begin{cases} -log(h_\theta(x)) & \text{if } y = 1 \\ -log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

Note that Cost=0, if y=1, $h_\theta(x) = 1$; but as $h_\theta(x) \to 0$, then $Cost \to \infty$. This proposition captures the intuition that if $h_\theta(x) = 0$, predict $P(y = 1 \mid x; \theta)$, but y ends up being 1, we will penalize the learning algorithm by very large cost.

6.5 Simplified Cost Function and Gradient Descent

Since y can only be either 0 or 1, we can simplify the cost function.

$$\begin{aligned} J(\theta) &= \frac{1}{m}\sum_{i=1}^{m} Cost\,(\,h_\theta(x^{(i)})\,,\,y^{(i)}) \\ &= \frac{-1}{m}\,[\,\sum_{i=1}^{m} y^{(i)}\,log\,h_\theta(x^{(i)}) \;+\; (1 - y^{(i)})\,log\,(\,1 - h_\theta(x^{(i)})\,)\,] \end{aligned} \tag{9}$$

Equation 9 is based on Maximum Likelihood Estimation.
A vectorized implementation is, for a design matrix $\mathbf{X}$:

$$\boxed{h = g(\mathbf{X}\theta)} \tag{10}$$

$$\boxed{J(\theta) = \frac{1}{m}(-y^T log(h) - (1 - y)^T log(1 - h))} \tag{11}$$

For gradient descent,we would want to $\min_\theta J(\theta)$:

Repeat {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

}

We can compute the partial derivative of $J(\theta)$, which is identical to that of linear regression:

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

However, in this case the hypothesis function $h_\theta(x) = \frac{1}{1+exp(-\theta^T x}$ has changed!

A vectorized implementation for this is:

$$\boxed{\theta := \theta - \frac{\alpha}{m} \mathbf{X}^T (g(\mathbf{X}\theta) - \mathbf{y}))} \tag{12}$$

6.6 Advanced Optimization

6.6.1 Taking a Step Back

If we take a step back, and consider essentially what tasks we are performing. We need to compute two things:

1. $J(\theta)$
2. $\frac{\partial}{\partial \theta_j} J(\theta)$

6.6.2 Optimization Algorithm

There exists other more sophisticated and faster ways to optimize θ instead of gradient descent; they often do not involve selecting learning rate α and are more efficient. However, these algorithms are harder to code by hand. It is suggested that we use libraries for such algorithms.

We can write a single function that returns both $J(\theta)$ (jVal) and $\frac{\partial}{\partial \theta_j} J(\theta)$ (gradient):

```
function [jVal, gradient] = costFunction(theta)
    jVal = [...code to compute J(theta)...];
    gradient = [...code to compute derivative of J(theta)...];
end
```

Then we can use octave's "fminunc()" optimization algorithm along with the "optimset()" function that creates an object containing the options we want to send to "fminunc()".

```
    options = optimset('GradObj', 'on', 'MaxIter', 100);
    initialTheta = zeros(2,1);
    [optTheta, functionVal, exitFlag] = fminunc(@costFunction,
        initialTheta, options);
```

We then give to the function "fminunc()" our cost function, our initial vector of theta values, and the "options" object that we created beforehand.

6.7 Multiclass Classification: One-vs-All

Now, let's extend the binary classification of data to multi-classes, i.e expanding our definition of y s.t. y={0, 1, . . . , n}. We will divide out problem into n+1 (0. . . n) binary classification problems. In each problem, we predict the probability that y is a memember of one of our class. We train a logistic regression classifier $h_\theta^{(i)}(x)$ ∀ i to predict y = i:

$$h_\theta^{(i)}(x) = P(y = i \mid x; \theta) \tag{13}$$

Figure 4 shows an example of the procedure of classifying three classes. We choose one class and then lump all the others into a single second class (hence the name One-vs-All). We apply the binary logisic regression repeatedly and use the hypothesis that returns the highest value.

$$prediction = \max_i \left(h_\theta^{(i)}(x) \right) \tag{14}$$

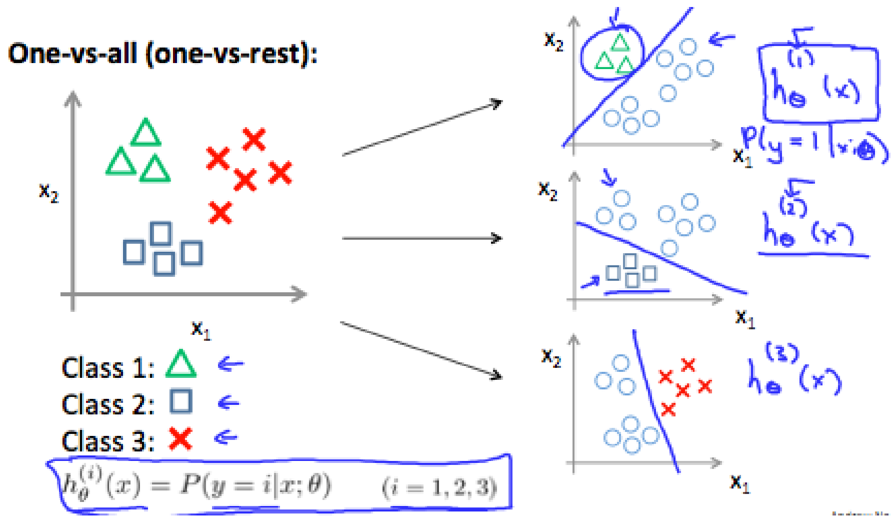


Figure 4: Example of Multiclass Logistic Regression

7 Regularization

7.1 The problem of overfitting

There are two types of errors in fitting functions to data, in which data shows the structure is not captured by the model. The terminology applies to both linear and logistic regression. Figure 5 shows an example of each fitting case.

1. Underfitting (high bias): when the form of our hypothesis function ($h_\theta(x)$) maps poorly to the trend of data. It is usually caused by a function that is either too simple or uses too little features.

2. Overfitting (high variance): when hypothesis function learns the training set very well hence fits the available data but does not generalize well to predict new data, i.e fitting too many details. It is usually caused by a complicated function that creates a lot of unneccessary curves and angles unrelated to the data.

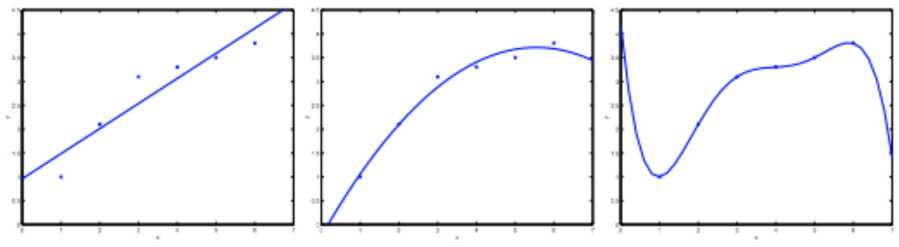


Figure 5: Three scenarios of fitting: underfit(left), good fit (middle), and overfit(right).

There are two main options to address the issue of overfitting:

1. Reduce the number of features
   - manually select which features to keep.
   - Use a model selection algorithm (later in the course).
2. **Regularization**
   - Keep all the features, but reduce the magnitude of parameters θ_j
   - Regularization worls well when we have a lot of slightly useful features. (Each contributes a bit to predict y)

7.2 Cost Function

7.2.1 Intuition

Suppose we have overfitting, we can reduce the weight that some of the terms in our function carry by penalizing the feature parameter with increased cost. Consider the following hypothesis function :

$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta x^3 + \theta x^4.$$

We would want to make the function more quadratic, which means we would like to reduce the influence of θ_3 and θ_4. Since our goal was to minimize the cost function $J(\theta)$, we could modify the original cost function

$$\min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000 \cdot \theta_3^2 + 1000 \cdot \theta_4^2.$$

This will force θ_3 and θ_4 to be close to zero, and make the original hypothesis function more quadratic.

7.2.2 Regularization

Now, we can take a step further and regularize all theta parameters:

$$\min_\theta \ [\frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2] + \lambda \sum_{j=1}^{n} \theta_j^2 \tag{15}$$

Here we are performing two separate operations which can be oberved as the two terms in Equation 15. The first term corresponds to “training the data”, and the second term relates to “keeping the parameters small”. The coefficient λ is the **regularization parameter** and determines the balance between the aforementioned two objectives. Note that if λ is too big ($\approx 10^{10}$), then all $\theta_j \approx 0$, except for θ_0 (the constant term). This makes $h_\theta \approx 0$ and defies the purpose of training and leads to underfitting (a flat horizontal line).

7.3 Regularized Linear Regression

7.3.1 Gradient Descent

We will modify the gradient descent function to separate out θ_0 from the rest of the parameters because we do not want to penalize θ_0.

repeat until convergence{

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha [(\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}) + \frac{\lambda}{m} \theta_j]$$

} , where $j \in \{1, 2, \ldots, n\}$

The above equation can be re-arranged to get the final form:

$$\boxed{\theta_j := \theta_j(1 - \alpha\frac{\lambda}{m}) - \frac{\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}} \tag{16}$$

The term $(1 - \alpha\frac{\lambda}{m})$ will always be less than 1. Intuitively, this reduces the parameter, then the rest of equation 16 carries the normal gradient descent.

7.3.2 Normal Equation

Recall from our previous normal equation (Equation 7), we have the design matrix $\mathbf{X}$ such that

$$\mathbf{X} = \begin{bmatrix} — & (x^{(1)})^T & — \\ — & (x^{(2)})^T & — \\ — & (x^{(3)})^T & — \\ & \vdots & \\ — & (x_m^T & — \end{bmatrix}$$

Now, to add in regularization to Equation 7, we get:

$$\boxed{\theta = ((\mathbf{X^T X}) + \lambda \cdot \mathbf{L})^{-1}\mathbf{x}^T y} \tag{17}$$

where $L \in \mathbb{R}^{(n+1)\times(n+1)}$

$$L = \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} \tag{18}$$

Supopose non-invertibility arises: $m \leq n$, i.e #examples is less than or equal to number of features, then using a $\lambda > 0$ in Equation 17 will resolve the non-invertibility.

7.4 Regularized Logistic Regression

7.4.1 Regularized Logistic Cost Function

We can modify our old logistic cost function (Equation 9) to apply regularization.

$$\boxed{J(\theta) = \frac{-1}{m}\sum_{i=1}^{m}[y^{(i)}\, log\, h_\theta(x^{(i)}) \;+\; (1 - y^{(i)})\, log\,(\,1 - h_\theta(x^{(i)})\,)] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2} \tag{19}$$

Note that the second sum in Equation 19 explicitly exludes the bias term θ_0.

7.4.2 Regularized Logistic Gradient Descent

The gradient descent is similar to that of linear regression; however note that the hypothesis function has been updated to Equation 8.

repeat until convergence{

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha [(\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}) + \frac{\lambda}{m} \theta_j]$$

}

8 Neural Networks: Representation

8.1 Non-linear Hypothesis

- Example: non-linear classification- logistic regression has lots of terms and not scalable($O(n^2), O(n^3)$).
- Application: computer vision
- Neural network is useful for **non-linear, large scale classification**.

8.2 Neurons and the brain

- Origin: Neuromorphic computing mimics how brain functions.
- Recent resurgence due to hardware advancement.
- The "one-learning hypothesis": there exists a single algorithm that the brain uses for generalized learning.
  - Neural re-wiring: wiring the auditory cortex to eyes, then the cortex learns how to *see*.

8.3 Model representation

Figure 6 shows a model of a biological neuron. The **dendrites** are the wires which receive input signal. The **axons** output the signal.

Neuron in the brain

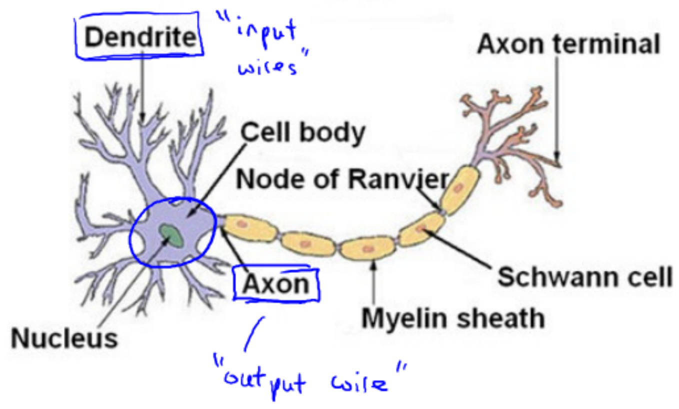


Figure 6: A biological neuron

8.3.1 Neural model: logistic unit

In our model:

- Dendrites: input features x_1, x_2, ..., x_n.
- Output: result of hypothesis function.
- x_0: bias unit (:= 1).
- Logistic function: $\frac{1}{1+exp(-\theta^T X)}$, referred to as the sigmoid(logistic) **activation** function.
- θ are referred to as **weights**.

Visually, a simplistic representation can be view as

$$[x_0\ x_1\ x_2] \rightarrow [\,] \rightarrow h_\theta(x) \tag{20}$$

The input nodes (layer 1, input layer) go into the another node (layer 2), which then outputs to hypothesis function (output layer).

In this example, we label the intermediate layers of nodes (between the input and output layers) $a_0^2, \ldots, a_n^2$: **activation units**. Definitions:

$\boxed{a_i^{(j)} = \text{“activation of unit i in layer j}}$

$\boxed{\Theta^{(j)} = \text{matrix of weights controlling function mapping from layer j to layer j+1.}}$

If we had one hidden layer, it would look like:

$$\boxed{[x_0\,x_1\,x_2\,x_3] \;\rightarrow\; [a_1^{(2)}, a_2^{(2)}, a_3^{(2)}] \;\rightarrow h_\theta(x)}$$

The value for each of the activation node is obtained as follows;

$$a_1^{(2)} = g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3)$$

$$a_2^{(2)} = g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3)$$

$$a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$$

$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(1)}a_0 + \Theta_{11}^{(1)}a_1 + \Theta_{12}^{(1)}a_2 + \Theta_{13}^{(1)}a_3)$$

Essentially, each layer j has its own **matrix of weights**, $\Theta^{(j)}$.

If network has s_j units in layer j and s_{j+1} units in layer j+1, then $\Theta^{(j)}$ will be of dimension $s_{j+1} \times (s_j + 1)$.

The $+1$ comes from the addition in $\Theta^{(j)}$ of the bias nodes, x_0 and $\Theta_0^{(j)}$.

In the above example, layer 2 has 3 units ($a_1^{(2)}, a_2^{(2)}, a_3^{(2)}$) and layer 1 has 3 units (not including the bias unit). Therefore the weight matrix $\Theta^{(1)}$ which maps layer 1 to layer 2 is of dimension $3 \times (3 + 1)$.

Another example: if layer 1 has 2 input nodes and layer 2 has 4 activation nodes- dim ($\Theta^{(1)}$) is going to be 4x3 where $s_j = 2$ and $s_{j+1} = 4$, so $s_{j+1} \times (s_j + 1) = 4 \times 3$.

8.3.2 Forward Propagation: Vectorized Implementation

Define a new variable: $z_k^{(j)}$ as the parameter for for the logistic function $g(z)$ such that:

$$a_1^{(2)} = g(z_1^{(2)})$$
$$a_2^{(2)} = g(z_2^{(2)})$$
$$a_3^{(2)} = g(z_3^{(2)})$$

Therefore, for layer j=2 and unit k:

$$z_k^{(2)} = \Theta_{k,0}^{(1)}x_0 + \Theta_{k,1}^{(1)}x_1 + \cdots + \Theta_{k,n}^{(1)}x_n$$

$$x = \begin{bmatrix} x_0 \\ x_1 \\ \cdots \\ x_n \end{bmatrix} \; z^{(j)} = \begin{bmatrix} z_1^{(j)} \\ z_2^{(j)} \\ \cdots \\ z_n^{(j)} \end{bmatrix}$$

We can further generalize by setting $\mathbf{x} = a^{(1)}$ and re-write the equation:

$$z^{(j)} = \Theta^{(j-1)}a^{(j-1)} \tag{21}$$

Dimension check:

- $\Theta^{(j-1)}$ is of dimension $s_j \times (n+1)$.
- $\mathrm{a}^{(\mathrm{j})}$ is a column vector with dimension $1 \times (j+1)$.

Thus the logistic function is applied element-wise to **z**:

$$a^{(j)} = g(z^{(j)}) \tag{22}$$

We then add the bias unit $a_0^{(j)} = 1$ to the activation matrix. If we propagate forward by one layer in Equation 21:

$$z^{(j+1)} = \Theta^{(j)} a^{(j)} \tag{23}$$

The last theta matrix $\Theta^{(j)}$ will have only one row which is multiplied by one column $a^{(j)}$ such that the result is a single scalar.Hence the final hypothesis output is:

$$h_\theta(x) = a^{(j+1)} = g(z^{(j+1)}) \tag{24}$$

8.4 Application - Logic Gate Synthesis

We can apply neural networks to predict various logic gates: AND, OR, XOR, NOR. The basic graph can be represented as :

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow [\ g(z^{(2)})\ ] \rightarrow h_\Theta(x)$$

8.4.1 AND Gate

Let the first theta matrix be:

$$\Theta^{(1)} = [\ -30\ \ 20\ \ 20\ ]$$

Table 2 outlines the logistic hypothesis output which represents an AND gate: output = 1 $\iff$ ($x_1 = 1$ and $x_2 = 1$). The intuition here in choosing the Θ parameters is that we want the sigmoid function evaluate to be positive only when both x_1 and x_2 are logic 1. Therefore, we assign the bias unit to a large negative value, such that the result of Θx is positive only when both the two other weights are added.

8.4.2 OR Gate

Similarly, Table 3 outlines the truth table for the OR function. We pick a parameter matrix:

$$\Theta^{(1)} = [\ -10\ \ 20\ \ 20\ ]$$

x_1	x_2	z	$h_\Theta(x) = g(z)$
0	0	-30	0
0	1	-10	0
1	0	-10	0
1	1	10	1

Table 2: Truth table of AND gate

x_1	x_2	z	$h_\Theta(x) = g(z)$
0	0	-10	0
0	1	10	1
1	0	10	1
1	1	30	1

Table 3: Truth table of OR gate

8.4.3 NOR Gate

Similarly, Table 4 outlines the truth table for the NOR function. We pick a parameter matrix:

$$\Theta^{(1)} = \left[\begin{array}{ccc} 10 & -20 & -20 \end{array}\right]$$

8.4.4 NOT Gate

For an inversion, we just need a single parameter x. Table 5 outlines the truth table for the NOT function. We pick a parameter matrix:

$$\Theta^{(1)} = \left[\begin{array}{cc} 10 & -20 \end{array}\right]$$

8.4.5 XNOR Gate

Now, we would like to synthesize the XNOR function (shown in Table 6. This requires a three level neural network. We can decompose the function XNOR:

$$\overline{x_1 \oplus x_2} = x_1 x_2 + \overline{x_1} \cdot \overline{x_2}$$

x_1	x_2	z	$h_\Theta(x) = g(z)$
0	0	10	1
0	1	-10	0
1	0	-10	0
1	1	-30	0

Table 4: Truth table of NOR gate

x	z	$h_\Theta(x) = g(z)$
0	10	1
1	-10	0

Table 5: Truth table of NOT gate

x_1	x_2	$a_1^{(2)}$	$a_2^{(2)}$	$h_\Theta(x)$
0	0	0	1	1
0	1	0	0	0
1	0	0	0	0
1	1	1	0	1

Table 6: Truth table of XNOR

Therefore, in the second layer we will computer the AND and NOR functions then apply OR to the two intermediate output in the third layer.

$$\Theta^{(1)} = [\ -30\ \ 30\ \ 20\ \ ]$$

$$\Theta^{(2)} = [\ -10\ \ 20\ \ 20\ \ ]$$

So:

$$a^{(2)} = g(\Theta^{(1)} \cdot x)$$
$$a^{(3)} = g(\Theta^{(2)} \cdot a^{(2)})$$
$$h_\Theta(x) = a^{(3)}$$

8.5 Multi-class Classification

For multi-class classification, our prediction will be a column vector with each element be of “whether the current item belongs to the class of that position”. For example, for a 4-class classification, an example output would be:

$$h_\Theta(x) = [0010]$$

9 Neural Networks: Learning

9.1 Cost Function

Define variables:

- L :total number of layers in the network.
- s_l: number of units (not counting bias unit) in layer l.

- K: number of output classes.

Recall for classifications, we have binary and multi-class:

1. Binary classification:
    - y = 0 or 1.
    - 1 output unit, i.e. $h_\Theta(x) \in \mathbb{R}$.
    - $\mathrm{S_L}$ = 1; K = 1.
2. Multi-class classification:
    - $y \in \mathbb{R}^K$
    - $\mathrm{S_L}$= K. K≥3.

Recall the cost function for regularized logistic regression in Equation 19, shown below:

$$J(\theta) = \frac{-1}{m} \sum_{i=1}^{m} [y^{(i)}\, log\, h_\theta(x^{(i)}) \; + \; (1 - y^{(i)})\, log\,(\,1 - h_\theta(x^{(i)})\,)] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$$

For neural networks, we will extend Equation 19 into a generalized form:

$$\begin{aligned} J(\Theta) = & \frac{-1}{m} \sum_{i=1}^{m} \sum_{k=1}^{K} [y_k^{(i)}\, log\, h_\theta(x^{(i)})_k \; + \; (1 - y_k^{(i)})\, log\,(\,1 - h_\theta(x^{(i)})_k\,)] \\ & + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} (\Theta_{j,i}^{(l)})^2 \end{aligned} \tag{25}$$

In the first part of Equation 25, we added a summation to account for multiple output nodes. Note:

- Double sum adds up logistic regression costs calculated for each cell in the output layer.
- Triple sum adds up the squares if all individuals Θs in the entire network.
- The i in the triple sum does not refer to the training example i !

9.2 Backpropagation Algorithm

- Backpropagation: neural-network terminology for minimizing cost function.
- Gradient Computation: need to computer $J(\Theta)$ and $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$

Given a training set { $(x^{(1)}, y^{(1)}) \ldots (x^{(m)}, y^{(m)})$}. Set $\Delta_{i,j}^{(l)} = 0$ ∀ l,i,j.

For all training examples t=1:m:

1. Set $a^{(1)} := x^{(t)}$
2. Perform forward propagation to computer all the nodes ($a^{(l)}$).
3. Using $y^{(t)}$, compute $\delta^{(L)} = a^{(L)} - y^{(t)}$. (Vectorized deviation of output units to correct values).
4. Backpropagate the error:

   $$\delta^{(l)} = ((\Theta^{(l)})^T \delta^{(l+1)}).* a^{(l)}.*(1 - a^{(l)})$$

   This equation makes use of the fact that the derivative of the sigmoid function:

   $$g'(z^{(l)}) = a^{(l)}.*(1 - a^{(l)})$$

5. Obtain the estimation of gradient ($\nabla J(\Theta)$). Intuitively, $\delta^{(l)}$ is the error for the activation unit in layer l: a^{l}. more formally, the delta values are the derivatives of the cost functions.
   It can be shown that

   $$\boxed{\frac{\partial}{\partial \Theta_{i,j}^{(l)}} J(\Theta) = a_j^{(l)} \cdot \delta_i^{(l+1)}}$$

   Hence, a vectorized implementation of the accumulated gradient is:

   $$\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)}(a^{(l)})^T$$

We then normalize and add regularization to obtain the gradient:

- $D_{i,j}^{(l)} := \frac{1}{m}(\Delta_{i,j}^{(l)} + \lambda \Theta_{i,j}^{(l)})$, if j $\neq 0$
- $D_{i,j}^{(l)} := \frac{1}{m}\Delta_{i,j}^{(l)}$, if j=0

And thus $\frac{\partial}{\partial \theta^{(l)}} = D^{(l)}$.

9.3 Gradient checking

- Purpose: Eliminates error from escaping. Assuring backpropagation is working as intended.
- Approx derivative as:

  $$\frac{\partial}{\partial \Theta_j} J(\Theta) \approx \frac{J(\Theta_1, \dots, \Theta_j + \epsilon, \dots, \Theta_n) - J(\Theta_1, \dots, \Theta_j - \epsilon, \dots, \Theta_n)}{2\epsilon}$$

- Compute the gradient approximation and compare with backpropagation(delta vector)
- Turn off gradient checking as this is computationally expensive.

Below is an implementation of gradient checking in MATLAB code:

```
epsilon = 1e-4;
for i = 1:n,
  thetaPlus = theta;
  thetaPlus(i) += epsilon;
  thetaMinus = theta;
  thetaMinus(i) -= epsilon;
  gradApprox(i) = (J(thetaPlus) - J(thetaMinus))/(2*epsilon)
end;
```

9.4 Random Initialization

- Initializing all theta weights to zero does not work. In backpropagation, all nodes will update to the same value repeatedly, creating **symmetry**.
- Symmetry breaking: initialize to values that range in [-ϵ, ϵ]

10 Advice for Applying Machine Learning

10.1 Deciding What to Try Next

Potential next steps:

1. Larger training data.
2. Smaller set of feature.
3. Additional features.
4. Polynomial features.
5. Increase λ.
6. Decrease λ.

Machine Learning Diagnostic: a test to run to gain insight on feasibility of techniques and how to optimize performance.

10.2 Evaluating Hypothesis: training/validation/test sets

10.2.1 Motivation with Test sets

We want to address the problem of overfitting: fits training examples very well (low error) but fails to generalize and hence not inaccurate on additional data. Thus, to evaluate the true accuracy of hypothesis, we randomly split the data into two sets: a **training set** (70%) and a **test set** (30%). The procedure :

1. Learn Θ and minimize $J_{train}(\Theta)$ using the training set

2. Compute test set error: $J_{test}(\Theta)$.

   (a) For linear regression:

$$J_{test}(\Theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} (h_\theta(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

   (b) For logistic regression:

$$J(\theta) = \frac{-1}{m_{test}} \sum_{i=1}^{m_{test}} (y_{test}^{(i)} log(h_\Theta(x_{test}^{(i)}) + (1 - y_{test}^{(i)}) log(1 - h_\Theta(x_{test}^{(i)}))$$

   (c) For classification, we first calculate the misclassification error.

$$err(h_\Theta(x), y) = \begin{cases} 1 & \text{if } (h_\Theta(x) \geq 0.5 \text{ \& } y = 0) \text{ or } (h_\Theta(x) \leq 0.5 \text{ \& } y = 1) \\ 0 & \text{if otherwise.} \end{cases} \tag{26}$$

   The average test error is thus:

$$\text{Test error} = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} err(h_\Theta(x), y) \tag{27}$$

10.2.2 Polynomial features: Train/Validation/Test model

- Computed cost is less than the generalization error: We trained our data on the training set to obtain Θ with different degrees of polynomial (d). We then choose d based on minimizing the test set.
- Problem: $J_{test}(\Theta)$ is likely to be an optimistic generalization error, since the parameter d is fit to the test data set.
- Solution: break down dataset into three sections:
  1. Training set (60%).
  2. Cross-validation set (20%).
  3. Test set (20%).

Procedure:

1. Optimize the parameters in Θ using the training set for each polynomial degree.
2. Find the polynomial degree d with the least error using the cross validation set.
3. Estimate the generalization error using the test set with $J_{test}(\Theta^{(d)})$, (d = theta from polynomial with lower error);

This way, the degree of the polynomial d has not been trained using the test set.

10.3 Diagnosing Bias vs Variance

- Degree of polynomial (d) and underfitting (high bias) / overfitting (high variance).
- Training errors tend to decrease as d increases.
- Cross validation error tends to form a convex curve with a minimum point.

Therefore, the key to distinguish between bias and variance is summarized in Figure X.

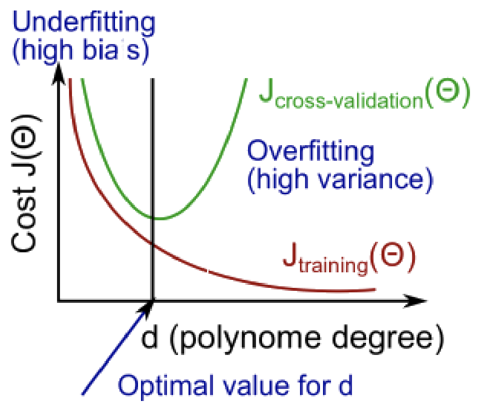


Figure 7: Error cost of cross-validation and training over degree of polynomial

1. **High bias (underfitting)**: both $J_{train}(\Theta)$ and $J_{CV}(\Theta)$ will be high. Thus: $J_{train}(\Theta) \approx J_{CV}(\Theta)$
2. **High variance (overfitting)**: *Low* $J_{train}(\Theta)$ and *high* $J_{CV}(\Theta)$. Thus: $J_{train}(\Theta) << J_{CV}(\Theta)$

10.4 Regularization and bias and variance

- Large λ (lower significance of Θ, heavy penalization so $h_\theta \approx 0$): high bias, underfit.
- Small λ (high significance of Θ): high variance, overfit.

Procedure to pick the right λ:

1. Create list of lambda.
2. Iterate through λs and learn/obtain Θ.
3. Compute cross-validation error ($J_{CV}(\Theta)$) using the learned Θ **without regularization** (i.e. $\lambda = 0$)
4. Select the best lambda and Theta pair and verify on test set. (Compute $J_{test}(\Theta)$.

10.5 Learning Curves

Plotting error over number of training examples.

10.5.1 High bias

1. Low training set size: low J_{train} and high J_{CV}.
2. Large training set size: high J_{train} and high J_{CV}.

Getting more training data will not help.

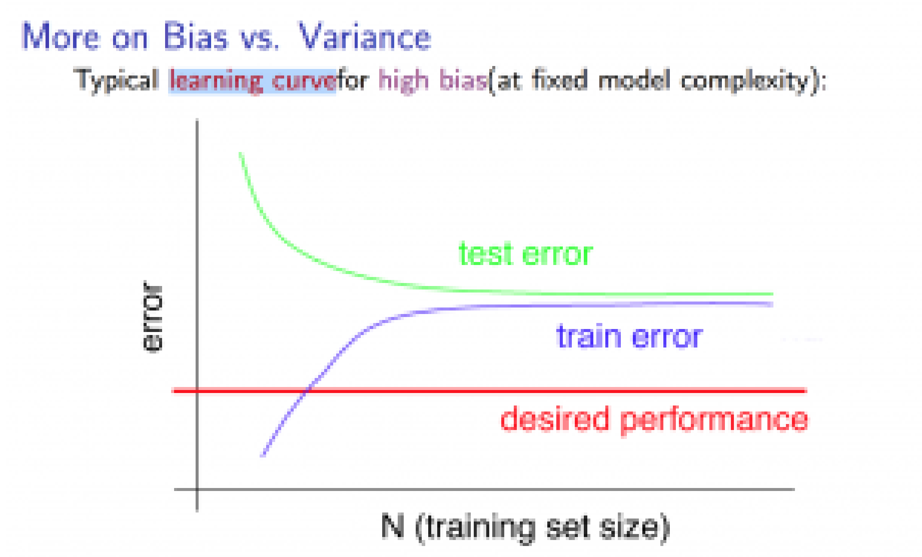


Figure 8: Learning curve for high bias

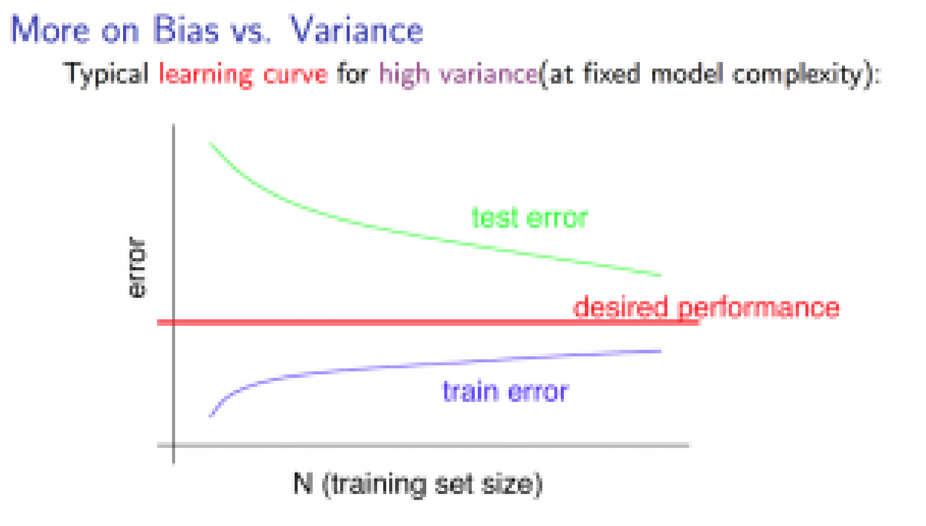
10.5.2 High variance

1. Low training set size: low J_{train} and high J_{CV}.
2. Large training set size: J_{train} increases and J_{CV} decreases.

Getting more training data will help.

10.6 Summary

1. Getting more training examples: Fixes high variance
2. Trying smaller sets of features: Fixes high variance
3. Adding features: Fixes high bias


More on Bias vs. Variance

Typical learning curve for high variance(at fixed model complexity):

Figure 9: Learning curve for high variance

4. Adding polynomial features: Fixes high bias
5. Decreasing λ: Fixes high bias
6. Increasing λ: Fixes high variance.

10.7 Neural Networks

1. Small neural network: fewer parameters $\implies$ prone to underfitting, but computationally cheaper.
2. Large neural network: more parameters $\implies$ prone to overfitting, computationally expensive. Use regularization to address overfitting.